

On phase-space integrals with Heaviside functions

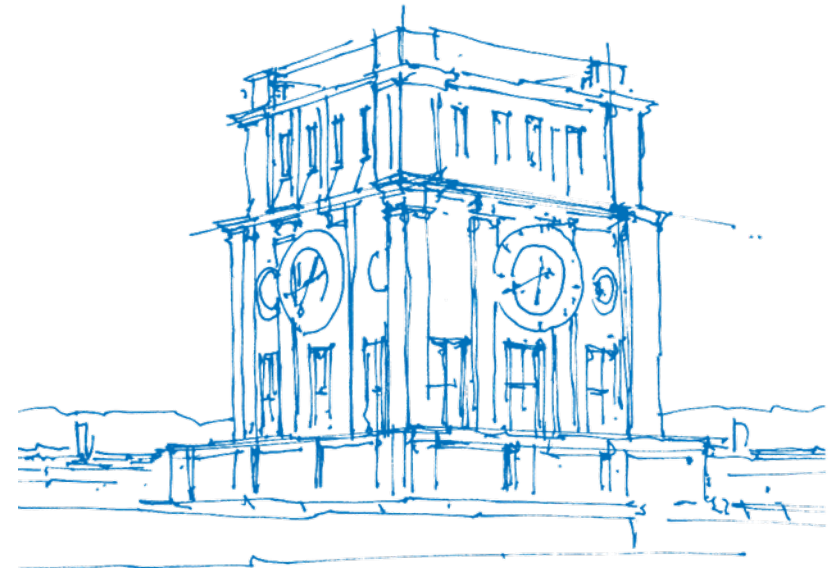
In collaboration with: D. Baranowski, K. Melnikov, A. Pikelner and C.-Y. Wang

Based on: 2111.13594 and 2204.094559

Maximilian Delto

Loopfest XXI

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TUM Uhrenturm

Fully differential predictions for LHC

[Chen et al. '22]

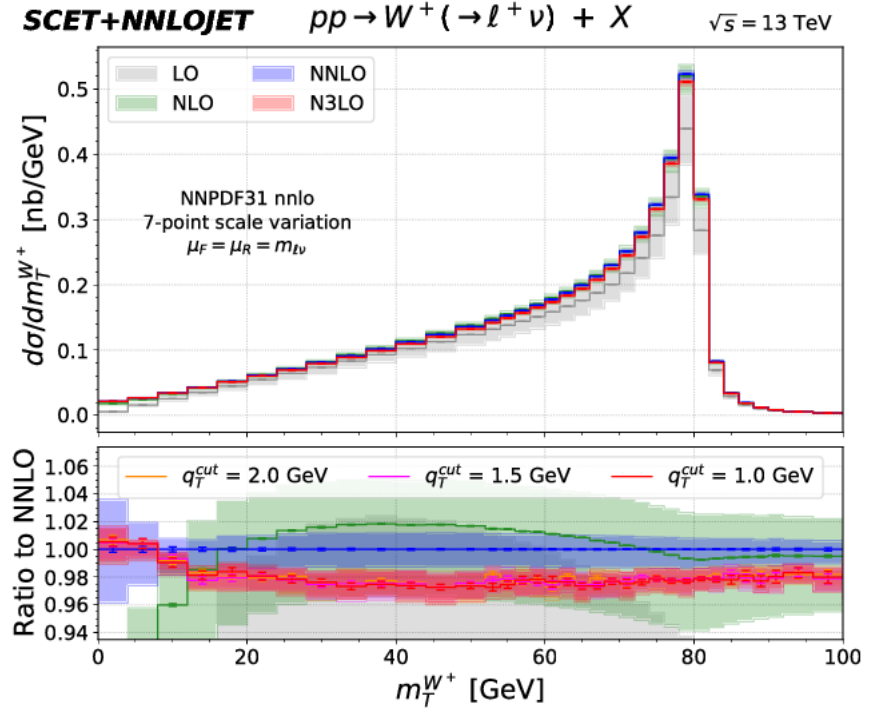
Fully-differential description of LHC cross sections for color singlet production has reached third order in perturbative QCD.

- ⇒ Higgs production [Chen et al. '21]
- ⇒ Drell-Yan [Chen et al. '22], [Chen et al. '22]

... as well as re-computation including resummation

- ⇒ Drell-Yan $N^4LL_p + N^3LO$ [Neumann et al. '22]

These computations are vital for precise studies at the LHC.



One (of many) challenges: **explicit** vs. **implicit** IR singularities

$$\left. \frac{d\sigma}{d\mathbf{O}} \right|_{\alpha_s} = 2 \Re \left[\underbrace{\left[\text{Diagram 1} \times \text{Diagram 2} \right]}_{\sim 1/\epsilon^2} \mathcal{F}_0 d\Phi_X + \left[\text{Diagram 3} + \text{Diagram 4} \right] \mathcal{F}_0^{(1)} d\Phi_{X+g} + \dots \right]$$

Handling IR divergences

Subtraction schemes

⇒ subtract and add back a term that approximates the divergent behavior

$$\mathcal{I} = \frac{f(0)}{n\epsilon} + \int_0^1 dx \frac{f(x) - f(0)}{x} + \mathcal{O}(\epsilon)$$

- ☺ local regularisation of divergences
- ☺ numerically stable
- ☹ complex construction, tedious to implement

for example

- CoLoRFull [Somogyi et al. '05]
- Antenna [Gehrmann-De Ridder et al. '05]
- STRIPPER [Czakon '10]
- Nested soft-collinear subtraction [Caola et al. '17]
- Local Analytic Sector Subtraction [Magnea et al. '18]
- ...

Slicing schemes

⇒ slice phase space into divergent and finite region

$$\mathcal{I} = \left[\frac{1}{n\epsilon} + \ln(\delta_{\text{cut}}) \right] f(0) + \int_{\delta_{\text{cut}}}^1 \frac{dx}{x} f(x) + \mathcal{O}(\delta, \epsilon)$$

- ☹ small cut-off leads to large numerical cancellations and requires precise control of f
- ☺ achievable at N3LO

for example

- q_T -slicing [Catani et al. '07]
- N -jettiness slicing [Boughezal et al. '15]
- ...

Other schemes

- projection-to-Born [Cacciari et al. '15]
- local unitarity [Capatti et al. '20]
- ...

Zero-jettiness slicing

Introduce

[see Riccardo's talk]

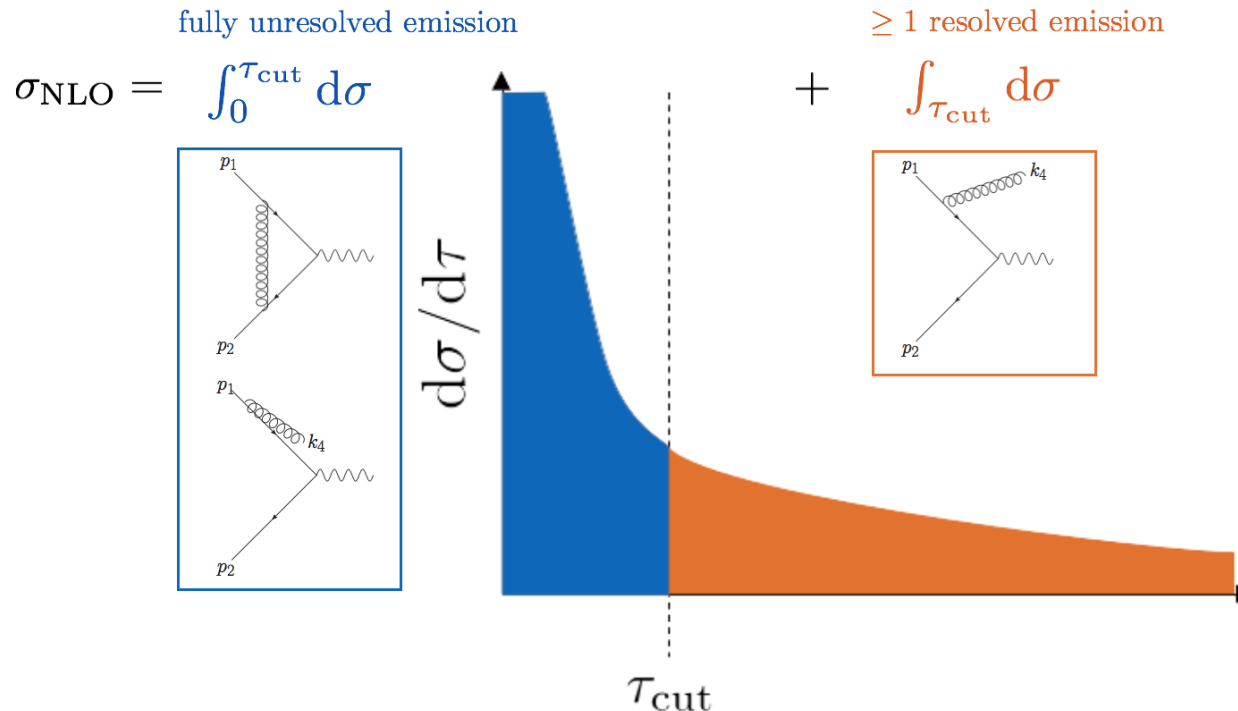
$$\tau = \sum_j \min_{q \in \{n, \bar{n}\}} \{q \cdot k_j\}, \quad q \cdot k_j = k_j^0 (1 \mp \cos \theta_j) \text{ for } q = n, \bar{n}$$

where $\tau = 0 \Leftrightarrow$ all emitted partons unresolved (soft/collinear to incoming partons).

Write cross-section as

$$\sigma_{\text{NLO}} = \int \frac{d\sigma}{d\tau} d\tau$$

and slice phase-space



Zero-jettiness factorization

The below-cut region factorizes [\[Stewart et al. '09\]](#)

$$d\sigma = B \otimes B \otimes S \otimes H \otimes d\sigma_{\text{Born}} + \mathcal{O}(\tau)$$

Beam function

- collinear emission off incoming partons
- known through N3LO
[\[Behring et al '19\]](#)
[\[Ebert et al. '20\]](#)
[\[Baranowski et al '22\]](#)

Soft function

- soft, non-collinear emission
- known through N2LO
[\[Kelley et al. '11\]](#)
[\[Monni et al. '11\]](#)
- RRV N3LO [\[Chen et al. '22\]](#)

Hard function

- contains virtual corrections

⇒ factorisation allows for explicit computation and cancellation of $1/\epsilon$ IR poles

⇒ remaining $\mathcal{O}(\epsilon^0)$ coefficient yields below-cut cross section

⇒ potential linear power corrections, see e.g. [\[Alekhin et al. '21\]](#)

Missing ingredient is the triple-real contribution to the soft function.

$$S^{(3)} = \int d\Phi_3 |J_{ggg}|^2 + \int d\Phi_3 |J_{gq\bar{q}}|^2$$

Three-gluon-emission contribution

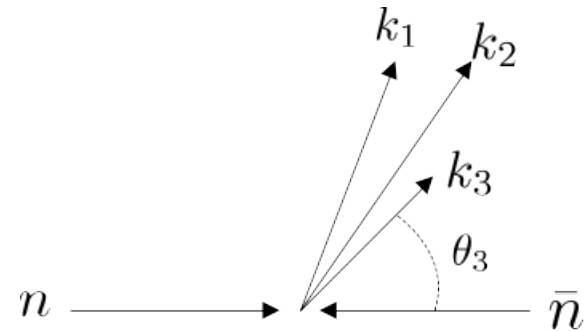
The maximally non-abelian 3g contribution

$$S^{ggg} \Big|_{C_A C_A^2} = 2 \int d\Phi_{\theta\theta\theta}^{nnn} |\mathbf{J}(k_1, k_2, k_3)|^2 + 6 \int d\Phi_{\theta\theta\theta}^{nn\bar{n}} |\mathbf{J}(k_1, k_2, k_3)|^2$$

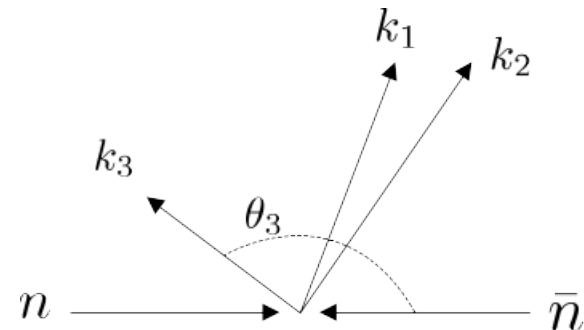
- triple-soft eikonal function $|\mathbf{J}|^2$ [Catani et al. '19] contains $\{q \cdot k_i, q \cdot k_{ij}, q \cdot k_{123}, k_i \cdot k_j, k_{123}^2\}$, $q = n, \bar{n}$
- zero-jettiness $\tau = \sum_j \min_{q \in \{n, \bar{n}\}} \{q \cdot k_j\}$

has two distinguishable configurations

$$1) d\Phi_{\theta\theta\theta}^{nnn} = [\widetilde{dk}] \delta[\tau - k_{123} \cdot n] \prod_{i=1}^3 \theta[k_i \cdot \bar{n} - k_i \cdot n]$$



$$2) d\Phi_{\theta\theta\theta}^{nn\bar{n}} = [\widetilde{dk}] \delta[\tau - k_{12} \cdot n - k_3 \cdot \bar{n}] \prod_{i=1}^2 \theta[k_i \cdot \bar{n} - k_i \cdot n] f_3(k_3 \cdot n - k_3 \cdot \bar{n})$$



where $[\widetilde{dk}] = \prod_{i=1}^3 d^d k_i \delta[k_i^2]$

Integration-by-parts relations

$$0 = \int \prod_{l=1}^L d^d k_l \frac{\partial}{\partial k_i^\mu} \left[q^\mu \prod_{n=1}^N D_n^{-\alpha_n} \right], \quad q \in \{k_1, \dots, k_L, p_1, \dots, p_E\}, \quad \alpha_n \in \mathbb{Z}, [\text{Chetyrkin, Tkachov '81}]$$

- set of linearly independent propagators $\{D_n\}$ defines topology uniquely
- IBP relations relate different integrals within a given topology

⇒ reduce given problem to minimal set of “master integrals” [AIR, FIRE, Reduze, LiteRed, Kira,..]

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$$(-2\pi i) \delta[q^2 - m^2] = \lim_{\sigma \rightarrow 0^+} \left[\frac{1}{q^2 - m^2 + i\sigma} - \frac{1}{q^2 - m^2 - i\sigma} \right] = \frac{1}{[q^2 - m^2]_c}$$

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2. θ -function:

Parametric representation

[Caola et al. '18] [Angeles-Martinez et al. '18]

[Bizon et al. '20] [Baranowski '20]

$$\theta[b - a] = \int_0^1 dz \delta[z \cdot b - a] \quad b, a, b > 0$$

[Chen '20]

$$(2\pi i) \theta[D] = \int_{-\infty}^{+\infty} dx \frac{e^{ixD}}{x + i0^+}$$

Integration-by-parts relations

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Extended notion of IBPs

[Baranowski et al. '21]

$$\frac{\partial}{\partial k} \{g(k) \theta[f(k)]\} = \overbrace{g' \theta}^{\text{hom}} + \overbrace{g \delta f'}^{\text{inhom}}$$

- ☹ proliferation of topologies
- ☹ manual generation of IBP identities
- ☺ no auxiliary integration

(see also [Luo et al. '19])

Integration-by-parts - example @ NNLO

$$\int \frac{d\Phi_{\theta\theta}^{nn}}{(k_2 n)(k_1 \bar{n})(k_{12} \bar{n})}, \quad d\Phi_{\theta\theta}^{nn} = [\widetilde{dk}] \delta[\tau - k_{12} n] \theta[k_1 \bar{n} - k_1 n] \theta[k_2 \bar{n} - k_2 n]$$

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$$\int \frac{d^d k_1 d^d k_2 \theta(k_1\bar{n} - k_1n) \theta(k_2\bar{n} - k_2n)}{[(k_1^2)(k_2^2)(\tau - k_{12}n)]_c (k_2n)(k_1\bar{n})(k_{12}\bar{n})} = \mathcal{T}_{1,1,1,0,1,1,1}^{\text{ex}}$$

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$$0 = [(d-4) - 7^+ 6^- - 3^+ 5^- + 3^+] \mathcal{T}_{1,1,1,0,1,1,1}^{\text{ex}} + \int d^d k_1 d^d k_2 [k_1^\mu (\bar{n} - n)_\mu \delta(k_1\bar{n} - k_1n)] \times \frac{\theta(k_2\bar{n} - k_2n)}{(k_1^2)(k_2^2)(\tau - k_{12}n)(k_2n)(k_1\bar{n})(k_{12}\bar{n})}$$

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⇒ “conventional” IBP relation

Integration-by-parts - example @ NNLO

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⇒ additional inhomogeneous term that requires **partial fraction decomposition**

Integration-by-parts - example @ NNLO

$$\underbrace{\mathcal{T}_{1,1,1,0,1,1,1}^{\text{ex}} = \int \frac{d\Phi_{\theta\theta}^{nn}}{(k_2 n)(k_1 \bar{n})(k_{12} \bar{n})}}_{\text{topology with } 2\theta\text{-functions}}, \quad d\Phi_{f_1 f_2}^{nn} = \widetilde{[dk]} \delta[\tau - k_{12} n] f_1[k_1 \bar{n} - k_1 n] f_2[k_2 \bar{n} - k_2 n]$$

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- because of inhomogeneous terms ($\sim \partial_k \theta$), we need new type of topologies:
 - come from all possible ways of replacing $\theta \rightarrow \delta$
 - fall into a hierarchical structure: $\{\theta\theta\} \xrightarrow{\partial_k \theta} \{\delta\theta, \theta\delta\} \xrightarrow{\partial_k \theta} \{\delta\delta\}$
 - relations for $\delta\delta$ topologies have no inhomogeneous terms
- feed relations to Kira \oplus FireFly [Maierhöfer et al. '17][Klappert et al. '19] (“user-defined equations”)

Integration-by-parts - example @ NNLO

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Reduction ✓ Master integrals X

Master integral computation - example @ NNLO

- consider

$$I_{4,\delta\theta}^{nn} = \int \frac{d\Phi_{\delta\theta}^{nn}}{(k_1 k_2)(k_2 n)(k_{12} \bar{n})}$$

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- expand with HypExp [Huber et al. '05] & integrate with HyperInt [Panzer '14]

$$I_{4,\delta\theta}^{nn} \Big|_{\tau \rightarrow 1} = \frac{2}{\varepsilon^2} + \frac{\pi^2}{3} - \frac{17\pi^4 \varepsilon^2}{90} + \varepsilon^3 [-6\pi^2 \zeta_3 - 26\zeta_5] - \varepsilon^4 \left[\frac{193\pi^6}{810} + 64\zeta_3^2 \right] + \mathcal{O}(\varepsilon^5)$$

Complications for three-gluon emission

General complexity

- more “level”: $\theta\theta\theta$, $\delta\theta\theta$, $\theta\delta\theta$, $\theta\theta\delta$, ...
- $\mathcal{O}(400)$ topologies
- integral relations

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Rapidity divergences

- known to appear for certain observables (e.g. q_T) in the limit of large rapidity
- only cancel in *soft+collinear*
- obey a rapidity renormalisation-group formalism [\[Chiu et al.\]](#)

in case of zero jettiness

- ⇒ we find individual integrals that are not regulated dimensionally
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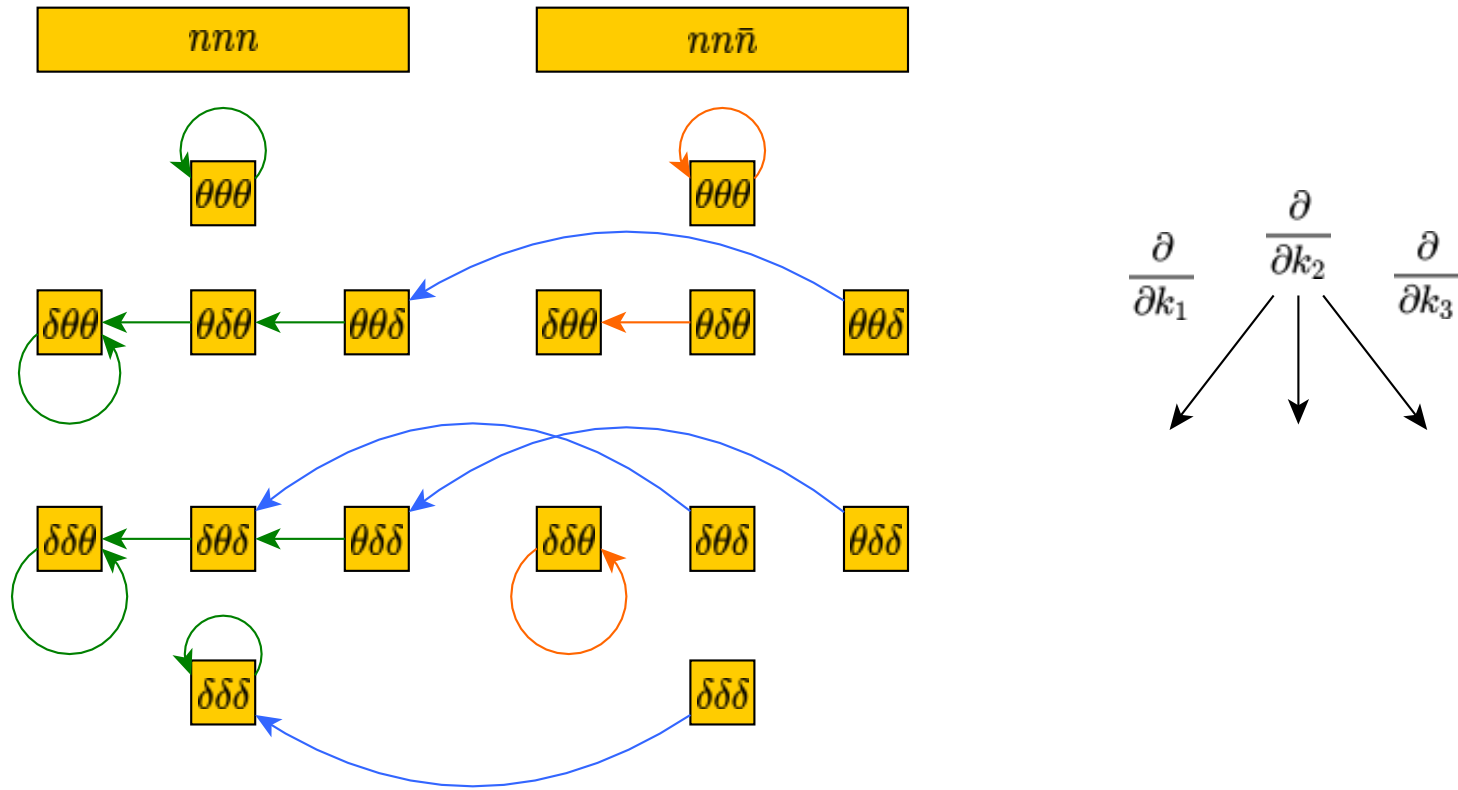
Master integrals

- more complicated master integrals
- ⇒ resort to numerical calculation and PSLQ reconstruction

Integral relations at N3LO

$$d\Phi_{f_1 f_2 f_3}^{nnn} \sim \delta[\tau - k_1 \cdot n - k_2 \cdot n - k_3 \cdot n] f_1(k_1 \cdot \bar{n} - k_1 \cdot n) f_2(k_2 \cdot \bar{n} - k_2 \cdot n) f_3(k_3 \cdot \bar{n} - k_3 \cdot n)$$

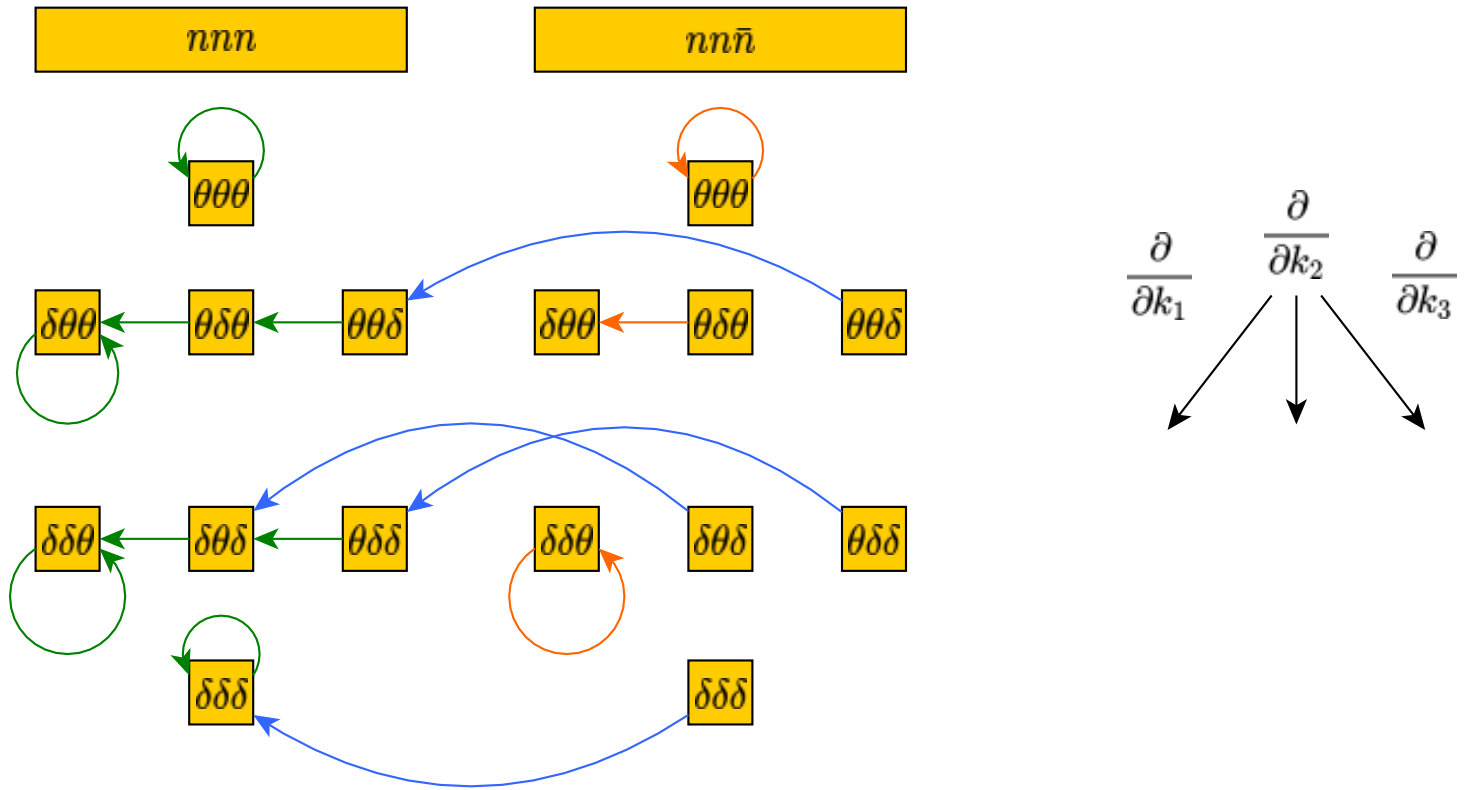
$$d\Phi_{f_1 f_2 f_3}^{nn\bar{n}} \sim \delta[\tau - k_1 \cdot n - k_2 \cdot n - k_3 \cdot \bar{n}] f_1(k_1 \cdot \bar{n} - k_1 \cdot n) f_2(k_2 \cdot \bar{n} - k_2 \cdot n) f_3(k_3 \cdot n - k_3 \cdot \bar{n})$$



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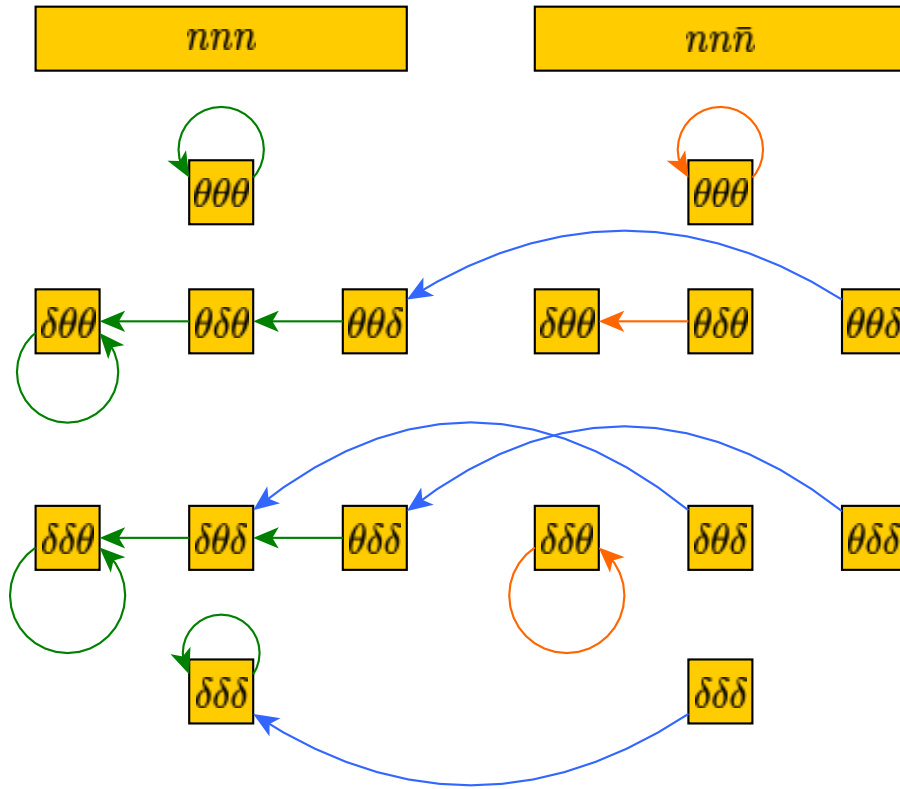
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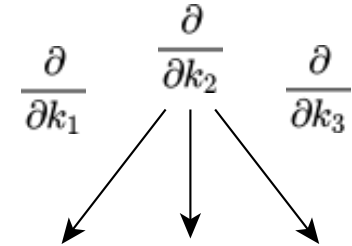
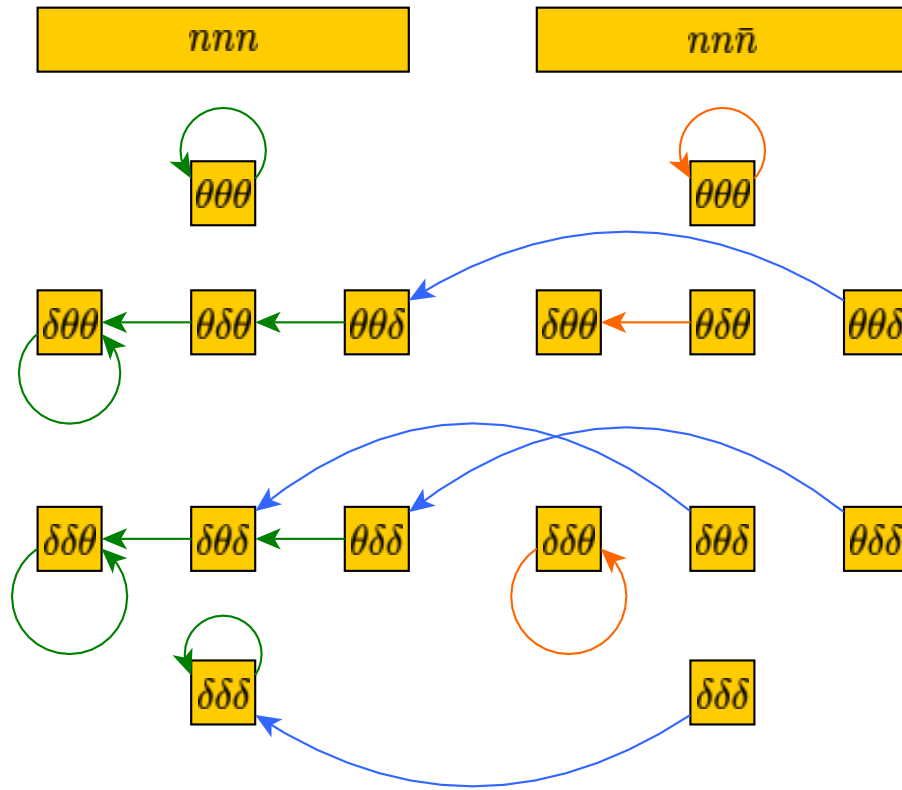


$$\frac{\partial}{\partial k_1} \quad \frac{\partial}{\partial k_2} \quad \frac{\partial}{\partial k_3}$$

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- modifies IBP relations (again)

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“ $\nu = 0$ ”-reduction
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- consider the following master integral

$$\bar{I}^{\nu} = \int \frac{d\Phi_{\theta\delta\theta}^{nnn,\nu}}{(k_1 k_3)(k_1 n)(k_{12} \bar{n})(k_3 \bar{n})}$$

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- consider the region $\beta_1 \sim \xi_1 \sim \xi_3 \sim \lambda \rightarrow 0$

$$\bar{I}^{\nu} = \int d\Omega \int \frac{d\lambda}{\lambda} \left(\frac{\lambda^2}{\lambda \lambda} \right)^{-\varepsilon} \lambda^{\nu} \times \dots \sim \frac{1}{\nu}$$

⇒ describes a situation where $g(k_2)$ is emitted in the transverse plane $k_2 n = k_2 \bar{n}$ and gluons $g(k_1), g(k_3)$ are very forward

Rapidity divergences at N3LO

Example

- consider the following master integral

$$\bar{I}^{\nu} = \int \frac{d\Phi_{\theta\delta\theta}^{nnn,\nu}}{(k_1 k_3)(k_1 n)(k_{12} \bar{n})(k_3 \bar{n})}$$

- employ Sudakov variables $k_i^{\mu} = \frac{1}{2} \left[\alpha_i n^{\mu} + \beta_i \bar{n}^{\mu} - 2\sqrt{\alpha_i \beta_i} e_i^{\perp} \right]$
- use $\delta[\alpha_2 - \beta_2]$
- introduce fraction $\xi_i = \beta_i / \alpha_i, i = 1, 3$

$$\bar{I}^{\nu} = \int d\Omega \int_0^1 \prod d\beta_i d\xi_1 d\xi_3 \left(\frac{\beta_1^2 \beta_3^2}{\xi_1 \xi_3} \right)^{-\varepsilon} \frac{\beta_2^{-2\varepsilon} \delta[1 - \beta_{123}] (\beta_1 \beta_2 \beta_3)^{\nu}}{(\xi_1 + \xi_3 - 2\sqrt{\xi_1 \xi_3} e_1^{\perp} e_2^{\perp}) \beta_1 (\beta_1 + \xi_1 \beta_2) \beta_3}$$

- consider the region $\beta_1 \sim \xi_1 \sim \xi_3 \sim \lambda \rightarrow 0$

$$\bar{I}^{\nu} = \int d\Omega \int \frac{d\lambda}{\lambda} \left(\frac{\lambda^2}{\lambda \lambda} \right)^{-\varepsilon} \lambda^{\nu} \times \dots \sim \frac{1}{\nu}$$

⇒ describes a situation where $g(k_2)$ is emitted in the transverse plane $k_2 n = k_2 \bar{n}$ and gluons $g(k_1), g(k_3)$ are very forward

⇒ $1/\nu$ -pole gets multiplied with reduction coefficient $c \sim \nu$

Master integrals at N3LO

Divide according to propagator $k_{123}^2 = 2[k_1k_2 + k_1k_3 + k_2k_3]$

- without k_{123}^2 : compute along the lines discussed for NNLO

$$\sim \int \frac{1}{(k_1k_2)(k_1k_3) \dots}$$

- with k_{123}^2 : difficult to compute analytically

Numerical computation of MI (see also [\[Liu et al. '17\]](#))

- add parameter m^2 to ‘complicated’ propagator

see also [\[Henn et al. '13\]](#)

$$I = \int \frac{d\Phi_{f_1f_2f_3}^v}{[k_{123}^2] \dots} \longrightarrow J = \int \frac{d\Phi_{f_1f_2f_3}^v}{[k_{123}^2 + m^2] \dots}$$

- using the IBP technology for θ -functions, derive differential equation

$$\partial_{m^2} J = \widehat{K} J$$

- compute boundary conditions in $m^2 \rightarrow \infty$, where the “bad” propagator simplifies
- solve differential equation numerically, compute the limit $m \rightarrow 0$, and recover I from Taylor-branch c_{000} in

$$J = \sum c_{n_1n_2n_3} (m^2)^{n_1+n_2\epsilon} \ln^{n_3}(m^2)$$

- result with 2000 digits, allows to reconstruct analytic expression with PSLQ

Results

$$\begin{aligned}
 S_3^{nn\bar{n}} = & \frac{24}{\varepsilon^5} + \frac{308}{3\varepsilon^4} + \frac{1}{\varepsilon^3} \left(-12\pi^2 + \frac{3380}{9} \right) + \frac{1}{\varepsilon^2} \left(-1000\zeta_3 + \frac{440\pi^2}{9} + \frac{10048}{9} \right) \\
 & + \frac{1}{\varepsilon} \left(-\frac{2377\pi^4}{45} + \frac{440\zeta_3}{3} + \frac{7192\pi^2}{27} + \frac{253252}{81} \right) \\
 & + \left(-28064\zeta_5 + \frac{1972\zeta_3\pi^2}{3} - \frac{638\pi^4}{15} + 4224\text{Li}_4\left(\frac{1}{2}\right) + 3696\zeta_3 \ln(2) - 176\pi^2 \ln^2(2) + 176\ln^4(2) \right. \\
 & + \frac{13208\zeta_3}{3} + \frac{78848\pi^2}{81} + 96\ln(2) + \frac{1925074}{243} \left. \right) \\
 & + \varepsilon \left(2304 \zeta_{-5,-1} - 4464\zeta_5 \ln(2) + 25784\zeta_3^2 - \frac{67351\pi^6}{567} - 6336G_R(0,0,r_2,1,-1) \right. \\
 & - 6336G_R(0,0,1,r_2,-1) - 3168G_R(0,0,1,r_2,r_4) - 6336G_R(0,0,r_2,-1) \ln(2) + \frac{268895\zeta_5}{3} \\
 & - 45056\text{Li}_5\left(\frac{1}{2}\right) - 45056\text{Li}_4\left(\frac{1}{2}\right) \ln(2) + 176\text{Cl}_4\left(\frac{\pi}{3}\right) \pi - 1056\zeta_3 \text{Li}_2\left(\frac{1}{4}\right) - 3982\zeta_3\pi^2 \\
 & - 21824\zeta_3 \ln^2(2) + 2112\zeta_3 \ln(2) \ln(3) - 1584\text{Cl}_2^2\left(\frac{\pi}{3}\right) \ln(3) - \frac{4400\text{Cl}_2\left(\frac{\pi}{3}\right) \pi^3}{27} + \frac{88\pi^4 \ln(2)}{45} \\
 & - \frac{616\pi^4 \ln(3)}{27} + \frac{11264\pi^2 \ln^3(2)}{9} - \frac{22528 \ln^5(2)}{15} + 8576\text{Li}_4\left(\frac{1}{2}\right) + 7504\zeta_3 \ln(2) + \frac{4174\pi^4}{27} \\
 & - \frac{1072\pi^2 \ln^2(2)}{3} + \frac{1072 \ln^4(2)}{3} + \frac{554032\zeta_3}{27} - 32\pi^2 \ln(2) + \frac{730378\pi^2}{243} - 384 \ln^2(2) + 832 \ln(2) \\
 & \left. + \frac{1408681}{81} + \sqrt{3} \left(192 \Im \left\{ \text{Li}_3 \left(\frac{\exp(i\pi/3)}{2} \right) \right\} + 160\text{Cl}_2\left(\frac{\pi}{3}\right) \ln(2) - 16\pi \ln^2(2) - \frac{560\pi^3}{81} \right) \right) + \mathcal{O}(\varepsilon^2)
 \end{aligned}$$

- most master integrals for $nn\bar{n}$ -configuration computed, checks in progress

One-jettiness @ NLO

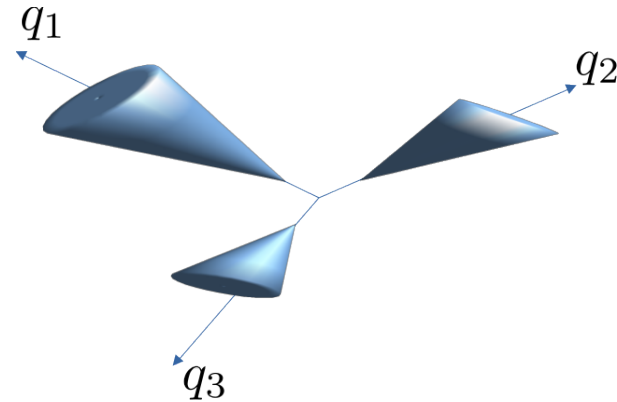
$$S = \int d^{d-1}k \sum_{i,j} \mathbf{T}_i \mathbf{T}_j \frac{q_i \cdot q_j}{(q_i \cdot k)(q_j \cdot k)} \delta[\tau - k \cdot q_1] \theta[k \cdot (q_2 - q_1)] \theta[k \cdot (q_3 - q_1)]$$

function of two angular ratios

$$x_1 = \frac{y_{12}}{y_{23}}, \quad x_2 = \frac{y_{13}}{y_{23}}$$

where

$$y_{ij} = \frac{q_i \cdot q_j}{E_i E_j}$$



six master integrals, canonical basis [Henn '13]

$$d\mathbf{J} = \varepsilon \sum_{\omega \in \mathcal{A}} d\log(\omega) \mathbf{J}$$

$$\mathcal{A} = \left\{ x_1, x_2, 1 - x_1, 1 - x_2, \lambda(1, x_1, x_2), \sqrt{\lambda(1, x_1, x_2)} + x_1 - x_2 - 1, \sqrt{\lambda(1, x_1, x_2)} - x_1 + x_2 - 1 \right\}$$

boundary conditions from equal-angle limit

$$y_{ij} = 1$$

$$J_2 \sim \frac{\Gamma(2 - 2\varepsilon)}{\Gamma^2(1 - \varepsilon)} + \frac{2^{-2\varepsilon}}{\pi} {}_2F_1 \left[\left\{ \frac{1}{2} - \varepsilon, \frac{1}{2} + \varepsilon \right\}, \left\{ \frac{3}{2} - \varepsilon \right\}; \frac{1}{4} \right]$$

(numerical computations through N2LO [Jouttenus et al. '11] [Boughezal et al. '15] [Campbell et al. '17])

Conclusion

extended notion of IBP relations & reverse unitarity

- enables us to reduce phase-space integrals that contain **Heaviside functions** to master integrals
- provides the means to derive differential equations, which we solve numerically

⇒ with this, we computed the same-hemisphere configuration (nnn) for three-gluon emission of the zero jettiness function

Outlook for zero-jettiness

- missing master integrals with k_{123}^2 -propagator in configuration $nn\bar{n}$ to finish ggg contribution
- other contributions are
 - RRR: $gq\bar{q}$ -emission: only reduction, master integrals identical
 - RRV: one-loop corrections to gg - and $q\bar{q}$ -emission: re-compute [\[Chen et al. '22\]](#)
 - RVV: two-loop correction to g -emission

General outlook

- extension to 1-jettiness under investigation
 - analytic structure, regularity conditions, ...
- other phase-space integrals containing Heaviside functions (soft counter terms in subtraction schemes, ...)